Topological Melting in Networks of Granular Materials

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Abstract

Granular materials represent a vast category of particle conglomerates with many areas of industrial applications. Here we represent these materials by graphs which capture their topological organization and ordering. Then, using the communicability function–a topological descriptor representing the thermal Green function of a network of harmonic oscillators–we prove the existence of a universal topological melting transition in these graphs. This transition resembles the melting process occurring in solids. We show here that crystalline-like granular materials melts at lower temperatures and display a sharper transition between solid to liquid phases than the random spatial graphs, which represent amorphous granular materials. In addition, we show the evolution mechanism of melting in these granular materials. In the particular case of crystalline materials the process starts by melting a central core of the crystal which then growth until the whole material is in the liquid phase. We provide experimental confirmation from published literature about this process.

1 Introduction

Melting–the phase transition in which a solid is transformed into a liquid–is a fundamental physical process of elements, substances and materials, which results from the application of heat or pressure to the substance [5, 2]. One of the most successful criteria for explaining melting at the microscopic level was developed by Lindemann in 1910 [15]. According to Lindemann criterion [15, 14], melting is caused by vibrational instability in the crystal lattice, which eventually makes that the amplitude of the vibration becomes so large that the atoms collide with their nearest neighbors, disturbing them and initiating the melting. Then, every substance is characterized by a melting point, which is the temperature at which such process starts. A crystal can be represented by a regular lattice [20] in which atoms are the nodes and interactions between atoms are the edges of a simple graph. It is then easy to set up a vibrational model on this graph by considering it as a ball-and-spring system and studying the change of state in it as a result of raising the temperature using the Lindemann criterion [15].

The use of graphs and networks to represent many granular materials has triggered their relevance as an object of study in this area of research [19]. Here we understand "granular materials" as a wide concept which include for instance, granular crystals [21, 23], microsphere monolayers [13], soft glassy materials [3], colloidal crystals [28], among others [17]. An important area of research in the study of the graph-representation of these granular materials is related to the robustness of these networks to the external stresses to which they may be submitted to [19]. For instance, Walker and Tordesillas [27] have studied the evolution of deformations in granular material networks under axial strain. In their work they have found that measures related to the communicability function of networks [9, 10] perform very well in describing such deformations. If we consider that the corresponding network represents a system of balls and springs submerged into a thermal bath at a given inverse temperature $\beta = (k_B T)^{-1}$ where k_B is the Bolztmann constant [10], the communicability function acquires the interpretation of being the thermal Green's function of the network [10]. It represents the capacity of a node to transmit a perturbation at a given β to another node of the network [10].

Here we consider a Lindemann-like model for the melting of granular networks. That is, we consider a vibrational model of nodes in a granular network based on the communicability function. Then, we prove analytically the existence of a universal phase transition in the communicability structure of every simple graph, which resembles the melting process occurring in materials. We discovered that, similar to crystalline and amorphous solids, regular and regular-like graphs "melt" at lower temperatures and display a sharper transition between connected to disconnected structures than the random spatial graphs, which resemble amorphous granular materials.

2 Preliminaries

Here we shall present some definitions, notations, and properties associated with networks to make this work self-contained. We will use indistinctly the terms networks and graphs across the paper. Here we consider only simple, undirected graphs $\Gamma = (V, E)$ with n nodes (vertices) and m edges. The notation used in the paper is the standard in network theory and the reader is referred to the monograph [7] for details. An important concept to be used across this paper is the one of walks. A *walk* of length k in Γ is a set of nodes $i_1, i_2, \ldots, i_k, i_{k+1}$ such that for all $1 \leq l \leq k$, $(i_l, i_{l+1}) \in E$. A *closed walk* is a walk for which $i_1 = i_{k+1}$. A *path* is a walk with no repeated nodes. A graph is *connected* if there is a path connecting every pair of nodes. Let A be the adjacency matrix of the graph Γ. For simple graphs A is symmetric and thus its eigenvalues are real, which we label here in non-increasing order:

$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. We will consider the spectral decomposition of $A\colon = U\Lambda U^T$, where Λ is a diagonal matrix containing the eigenvalues of A and $U = [\overrightarrow{\psi}_1, \ldots, \overrightarrow{\psi}_n]$ is orthogonal, where $\overrightarrow{\psi}_i$ is an eigenvector associated with λ_i. We consider here sets of orthonormalized eigenvectors of the adjacency matrix. Because the graphs considered here are connected, A is irreducible and from the Perron-Frobenius theorem we can deduce that $\lambda_1 > \lambda_2$ and that the leading eigenvector $\overrightarrow{\psi}_1$ can be chosen such that its components $\psi_1(p)$ are positive for all $p \in V$. It is known that $\left(A^k\right)_{pq}$ counts the number of walks of length k between p and q. The following result concerning the eigenvalue λ_2 is well-known in spectral graph theory. First, we define the following types of graphs. A *k-partite graph* is a graph whose vertices are partitioned into k different independent sets. An *independent set* is a set of nodes in the graph in which no pair of them are adjacent. A *complete k-partite graph* is a k-partite graph in which there is an edge between every pair of vertices from different independent sets.

Lemma 1. *([24]) Let $\Gamma = (V, E)$ be a connected graph and let $\lambda_1 > \lambda_2 \geq \lambda_3 \geq ... \geq \lambda_n$ be the eigenvalues of A. If the graph is not complete k-partite then $\lambda_2 > 0$.*

Two important results that we will use in the current work are the following. For the sake simplicity let us suppose that the vertices of the graph Γ are labeled as $V = \{1, 2, 3, \ldots, n\}$. For a given vector $\psi \in \mathbb{R}^n$, let $\mathscr{P}(\psi) = \{i : \psi(i) > 0\}$, $\mathscr{N}(\psi) = \{i : \psi(i) < 0\}$, and $\mathcal{O}(\psi) = \{i : \psi(i) = 0\}$, where $i \in V$, and let us denote by $\langle \mathscr{P}(\psi) \rangle$, $\langle \mathscr{N}(\psi) \rangle$ and $\langle \mathcal{O}(\psi) \rangle$ the subgraphs of Γ obtained by the nodes of the sets $\mathscr{P}(\psi)$, $\mathscr{N}(\psi)$ and $\mathcal{O}(\psi)$ respectively.

Lemma 2. *([22]) Let $\Gamma = (V, E)$ be a connected graph. Let A be its adjacency matrix, and let $\lambda_1 > \lambda_2 \geq \lambda_3 \geq ... \geq \lambda_n$ be the eigenvalues of A. Let $(r-1)$ be the multiplicity of λ_2 and let $\psi_2, \psi_3, ..., \psi_r$ be its corresponding eigenvectors. Suppose that $\cap_{j=2}^{r} \mathcal{O}(\psi_j) \neq \emptyset$. Then one of these two cases holds:*

1. No edge joins a vertex of $\mathscr{P}(\psi_j)$ to one of $\mathscr{N}(\psi_j)$, and $\langle \mathcal{P}(\psi_j) \cup \mathcal{N}(\psi_j) \rangle$ has r connected components.

2. Some edge joins a vertex of $\mathscr{P}(\psi_j)$ to one of $\mathscr{N}(\psi_j)$, and $\langle \mathcal{P}(\psi_j) \cup \mathcal{N}(\psi_j) \rangle$, $\langle \mathcal{P}(\psi_j) \rangle$

and $\langle \mathcal{N}(\psi_j) \rangle$ are all connected.

Lemma 3. *([25]) Let $\Gamma = (V, E)$ be a connected graph. Let $\lambda_2 > 0$ be the second largest eigenvalue of the adjacency matrix with multiplicity $(r-1)$. Then, there exist eigenvectors $\psi_2, \psi_3, ..., \psi_r$ corresponding to λ_2 such that the induced subgraphs generated by $\mathscr{P}(\psi_j) \cup \mathcal{O}(\psi_j)$ and $\mathcal{N}(\psi_j)$ $\forall j \in \{2, 3, \ldots, r\}$ are connected.*

Remark 4. Let ψ be the eigenvector corresponding to the eigenvalue λ_2. Then $\alpha\psi$, $\alpha \in \mathbb{R}$ is an eigenvector corresponding λ_2. If $\alpha > 0$, then $\mathscr{P}(\alpha\psi) = \mathscr{P}(\psi)$, $\mathscr{N}(\alpha\psi) = \mathscr{N}(\psi)$ and $\mathcal{O}(\alpha\psi) = \mathcal{O}(\psi)$. If $\alpha < 0$, then $\mathscr{P}(\alpha\psi) = \mathscr{N}(\psi)$, $\mathscr{N}(\alpha\psi) = \mathscr{P}(\psi)$ and $\mathcal{O}(\alpha\psi) = \mathcal{O}(\psi)$.

An important quantity for studying communication processes in networks has been defined as the communicability function [9, 11].

Definition 5. Let p and q be two nodes of Γ. The communicability function between these two nodes is defined as

$$G_{pq} = \sum_{k=0}^{\infty} \frac{\left(A^k\right)_{pq}}{k!} = \left(\exp\left(A\right)\right)_{pq} = \sum_{j=1}^{n} e^{\lambda_k} \psi_j(p)\psi_j(q).$$

It counts the total number of walks starting at node p and ending at node q, weighted in decreasing order of their length by a factor $\frac{1}{k!}$; therefore it is considering shorter walks more influential than longer ones. In this work we consider a generalization of the communicability function [10, 8] consisting of

$$G_{pq}\left(\beta\right) = \left(\exp\left(\beta A\right)\right)_{pq} = \sum_{j=1}^{n} e^{\beta\lambda_k} \psi_j(p)\psi_j(q),$$

where $\beta \geq 0$ is a parameter that weights homogeneously every edge of the graph Γ. Let us give a complete physical interpretation of the communicability function by considering the following model. Let us consider a network of quantum-harmonic oscillators, such as every node is a ball of mass m and two nodes are connected by a spring of strength constant ω (see [10] for details). We tie the network to the ground (to avoid translational movement) with

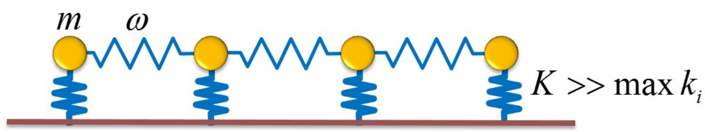


Figure 2.1: Illustration of the model used for deriving the thermal Green's function of a network of quantum harmonic oscillators.

springs of constant $K \gg \max k_i$ as illustrated in Figure 2.1 (we remind that k_i is the degree of the node i). The Hamiltonian describing the energy of this system is given by

$$\hat{H} = \sum_i \hbar\Omega \left(a_i^\dagger a_i + \frac{1}{2} \right) - \frac{\hbar\omega^2}{4\Omega} \sum_{i,j} \left(a_i^\dagger + a_i \right) A_{ij} \left(a_j^\dagger + a_j \right), \quad (2.1)$$

where A_{ij} are the elements of the adjacency matrix, $a_i^\dagger$ (a_i) are the annihilation (creation) operators, and $\Omega = \sqrt{K/m\Omega}$.

Let us submerge the network of quantum harmonic oscillators into a thermal bath with inverse temperature $\beta = (k_B T)^{-1}$, where k_B is a constant and T is the temperature. Then, the following result has been previously proved [10].

Theorem 6. [10] *The thermal Green's function of the network of quantum harmonic oscillators described by 2.1 is*

$$G_{pq}(\beta) = \exp(-\beta\hbar\Omega) \left(\exp \frac{\beta\hbar\omega^2}{2\Omega} A \right)_{pq}. \quad (2.2)$$

Remark 7. The thermal Green's function accounts for how the node p (respectively q) 'feels' a perturbation at node q (resp. p) due to thermal fluctuations in the bath.

When the temperature goes to infinity, the inverse temperature $\beta \to 0$, which means that every edge in the graph vanishes and the resulting graph is trivial, similar to a system of free particles. When the temperature goes to zero, the inverse temperature $\beta \to \infty$ indicating that an infinity number of edges are created between every pair of nodes connected in Γ; a situation analogous to a rigid solid.

3 Melting phase transition

Let us consider a connected graph with eigenvalues ordered as $\lambda_1 > \lambda_2 \geq \lambda_3 \geq ... \geq \lambda_n$. Let us then write the communicability function in the following way

$$\begin{aligned} G_{pq}(\beta) &= e^{\beta\lambda_1}\psi_1(p)\psi_1(q) + \left[\sum_{2\leq j\leq n} e^{\beta\lambda_j}\psi_j^+(p)\psi_j^+(q) + \sum_{2\leq j\leq n} e^{\beta\lambda_j}\psi_j^-(p)\psi_j^-(q)\right] \\ &+ \left[\sum_{2\leq j\leq n} e^{\beta\lambda_j}\psi_j^+(p)\psi_j^-(q) + e^{\beta\lambda_j}\psi_j^-(p)\psi_j^+(q)\right], \end{aligned}$$

where $\psi_j^+(p)$ ($\psi_j^-(p)$) means that the pth entry of the jth eigenvector is positive (negative). Let us consider the graph illustrated in Figure 3.1, where we show the corresponding eigenvectors of the adjacency matrix in a schematic way. The negative entries of the corresponding eigenvectors are illustrated like "vibrations" in the negative direction of the y-axis. Similarly for the positive entries, which are represented as vibrations in the positive direction of the y- axis. The magnitude of the vibrations are not represented for the sake of simplicity. The term $e^{\beta\lambda_1}\psi_1(p)\psi_1(q)$ represents the coordinated vibration of all nodes in the graph at the corresponding value of β (see Fig. 3.1). Then, we obtain the other vibrational terms for the pairs of nodes as: $\varDelta G_{pq}(\beta) = G_{pq}(\beta) - e^{\beta\lambda_1}\psi_1(p)\psi_1(q)$, which can also be expressed as

$$\varDelta G_{pq}(\beta) = \sum_{j\geq 2}^{in-phase} e^{\beta\lambda_j}\psi_j(p)\psi_j(q) - \left|\sum_{j\geq 2}^{out-of-phase} e^{\beta\lambda_j}\psi_j(p)\psi_j(q)\right|, \tag{3.1}$$

where the first term, which can be written as $\sum_{2\leq j\leq n} e^{\beta\lambda_j}\psi_j^+(p)\psi_j^+(q) + \sum_{2\leq j\leq n} e^{\beta\lambda_j}\psi_j^-(p)\psi_j^-(q)$, corresponds to the case when both nodes have the same sign in the corresponding eigenvector, and the second term, which can be written as $\sum_{2\leq j\leq n} e^{\beta\lambda_j}\psi_j^+(p)\psi_j^-(q) + e^{\beta\lambda_j}\psi_j^-(p)\psi_j^+(q)$, accounts for the cases in which the two nodes have different sign in the corresponding eigenvector. We notice that the second term is always negative and we use the modulus of it to express the term $\varDelta G_{pq}(\beta)$ as a difference. $\varDelta G_{pq}(\beta)$ accounts for the difference between the in- and out-of-phase vibrations of the corresponding pair of nodes.

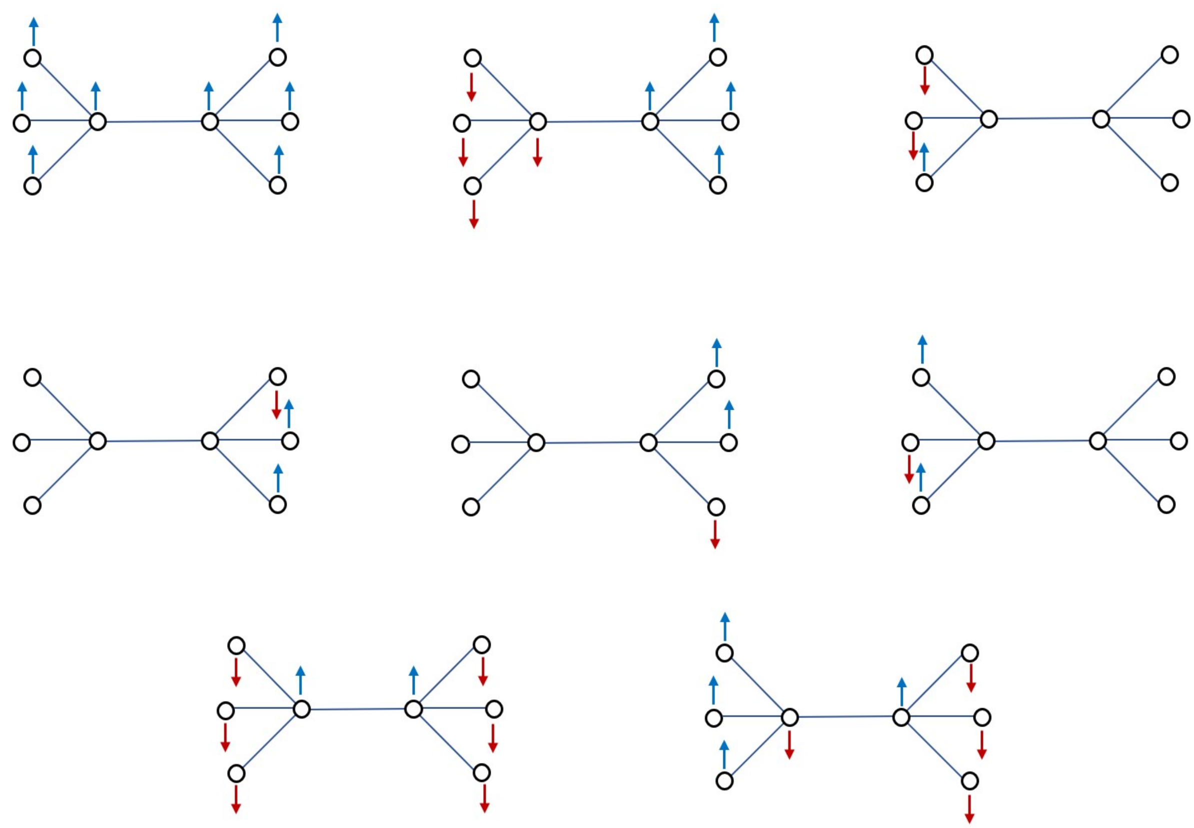


Figure 3.1: Illustration of the sign pattern of the eigenvectors in a simple graph. Only the signs of the eigenvector components are represented by blue (positive) and red (negative) arrows. The magnitudes of the eigenvector components are not represented.

Let us now reconnect with Lindemann criterion of melting [15]. According to Lindemann the average amplitude of thermal vibrations in crystals increases with the temperature up to a point in which the amplitude of vibration is so large that the atoms invade the space of their nearest neighbors and the melting starts. Lindemann criterion consists in considering that melting might be expected when the mean-square amplitude of vibrations exceed a certain threshold value [15]. Let us consider that in a graph Γ such threshold is given by $M(\mathit{\Gamma},\beta) = \max_{s \neq t \in V} \sum_{j=2}^{n} \psi_j(s)\,\psi_j(t)\,e^{\beta\lambda_j}$. That is, that melting starts in a given graph when the vibrations of the nodes p and q at a given temperature measured by $\Delta G_{pq}(\beta)$ exceed the value of the maximum vibration of any pair of nodes in that graph at the same temperature, $M(\mathit{\Gamma},\beta)$. We should notice that at a given temperature the terms $\mathit{\Delta} G_{pq}(\beta)$ and $M(\mathit{\Gamma},\beta)$ may be either positive or negative. Thus, in order to implement the Lindemann criterion on graphs we should sum both terms instead of having their difference,

$$\mathit{\Delta}\tilde{G}_{pq}(\beta) = M(\mathit{\Gamma},\beta) + \mathit{\Delta} G_{pq}(\beta). \tag{3.2}$$

Then, when $M(\mathit{\Gamma},\beta) > 0$ we have the following scenarios. If $\mathit{\Delta} G_{pq}(\beta) > 0$ then $\mathit{\Delta}\tilde{G}_{pq}(\beta)$ is always positive as it is the sum of two positive terms, indicating a *reinforcement* of the in-phase vibrations of the two nodes. If $\mathit{\Delta} G_{pq}(\beta) < 0$, then $\mathit{\Delta}\tilde{G}_{pq}(\beta) > 0$ if the difference between the in-phase and out-of-phase vibrations ($\mathit{\Delta} G_{pq}(\beta)$) does not overtake the maximum in-phase vibrations of any pair of nodes in the graph. Otherwise, $\mathit{\Delta}\tilde{G}_{pq}(\beta) < 0$, which indicates that the out-of-phase vibrations of these two nodes have overtaken not only their in-phase vibrations but also the maximum in-phase vibrations of any pair of nodes in the graph. In this last case we will say that the corresponding edge has been "melted". On the other hand, when $M(\mathit{\Gamma},\beta) < 0$, then also $\mathit{\Delta} G_{pq}(\beta) < 0$ which means that $\mathit{\Delta}\tilde{G}_{pq}(\beta) < 0$, and the edge necessarily "melts". Then, we will call $\mathit{\Delta}\tilde{G}_{pq}(\beta)$ the *graph Lindemann criterion*, having in mind that the melting will start when $\mathit{\Delta}\tilde{G}_{pq}(\beta) < 0$. Let us define the following representation of $\mathit{\Delta}\tilde{G}_{pq}(\beta)$ in the form of a new graph.

Definition 8. Let $\Gamma = (V, E)$ be a simple graph. The *communicability graph* $H(V, E', \beta)$ of

$\Gamma = (V, E)$ is the graph with the same set of nodes as Γ and with its edge set given by the following adjacency relation

$$A(H, \beta)_{p,q} = \begin{cases} 1 \text{ if } \mathit{\Delta}\tilde{G}_{pq}(\beta) \geq 0, \\ 0 \text{ if } \mathit{\Delta}\tilde{G}_{pq}(\beta) < 0. \end{cases} \tag{3.3}$$

In the communicability graph there could be edges connecting pairs of nodes which are not connected in the original graph Γ. In a similar way, there could be pairs of nodes not connected in $H(V, E', \beta)$ which correspond to edges in Γ (see further example). In other words, Γ is not necessarily a subgraph of $H(V, E', \beta)$. For instance, in Fig. 3.2 at $\beta = 1$ the two central nodes 1 and 5 of the graph are vibrating out-of-phase. However, because we do not have a temporal sequence of how the vibrations occurs there are also paths connecting 1 and 5 in which all the nodes vibrate in phase. This is the case of the paths 1-2-6-5, 1-4-8-5 and so forth. As a consequence of these paths the nodes 1 and 5 can be vibrating in-phase at some temporal stages of the process. For that reason we introduce the following definitions.

Definition 9. Let $\Gamma = (V, E)$ be a simple graph and let $H(V, E', \beta)$ be its communicability graph. Let p and q be two nodes of Γ. We say that there is a *Lindemann path* between the nodes p and q in Γ at a given value of β if there is a path connecting both nodes in the communicability graph $H(V, E', \beta)$. In this case we say that $\exists L_{p,q}$. Otherwise, we say that $\nexists L_{p,q}$.

We now define a graph that contain all the information about the in- and out-phase nature of the vibrations in a graph $\Gamma = (V, E)$.

Definition 10. Let $\Gamma = (V, E)$ be a simple graph and let $H(V, E', \beta)$ be its communicability graph. The *Lindemann graph* $F(V, E'', \beta)$ of Γ is the graph with the same set of vertices as Γ and edge set defined by the following adjacency relation

$$A(F, \beta)_{p,q} = \begin{cases} 1 \text{ if } (p, q) \in E \text{ and } \exists L_{p,q}, \\ 0 \text{ if } (p, q) \notin E \text{ or } \nexists L_{p,q}. \end{cases} \tag{3.4}$$

To illustrate the previously defined concepts we return to the tree with eight nodes and degree sequence 4,4,1,1,1,1,1,1 at different values of β illustrated in Fig. 3.2. For $\beta = 1$ the communicability graph has many more edges than the original tree Γ, but it also misses the central link connecting the nodes 1 and 5. When constructing the Lindemann graph we should observe that there is a path between every pair of nodes in the corresponding communicability graph, i.e., it is connected. Thus, the Lindemann graph consists of the same set of edges as the original graph. The Lindemann graph is represented by solid lines in the right panels of Fig. 3.2. When $\beta = 0.5$ the communicability graph consists of two cliques of four nodes each. Then, the Lindemann graph consists of all edges of Γ, except the central edge connecting the nodes 1 and 5, because there is no path connecting the two nodes of degree 4 in the communicability graph. At this value of β we can say that the melting of this graph has started because for (at least) one pair of nodes the out-of-phase vibrations have overcome the graph Lindemann criterion. Notice that for $\beta = 0.3$ the communicability graph has changed in relation to that for $\beta = 0.5$, but the Lindemann graphs are exactly the same due to the double conditions that need to be required for having an edge in these graphs. Finally, when $\beta = 0.2$ the communicability graph is formed by 8 isolated nodes and so is the Lindemann graph. At this point there is no communicability between any pair of nodes and the Lindemann graph is the trivial graph. In our physical metaphor, the graph is totally "melted".

In the Fig. 3.3 we have plotted the values of β versus the number of connected components of the Lindemann graph. At the point $\beta = 0.5$, marked in the plot with a fat arrow, there is a transition between a connected to a disconnected Lindemann graph. Let us call $\beta = \beta_c$ the melting temperature of this graph. The question that immediately emerges here is whether this phase transition is universal for any simple graph or not. In the next section we respond positively to this question.

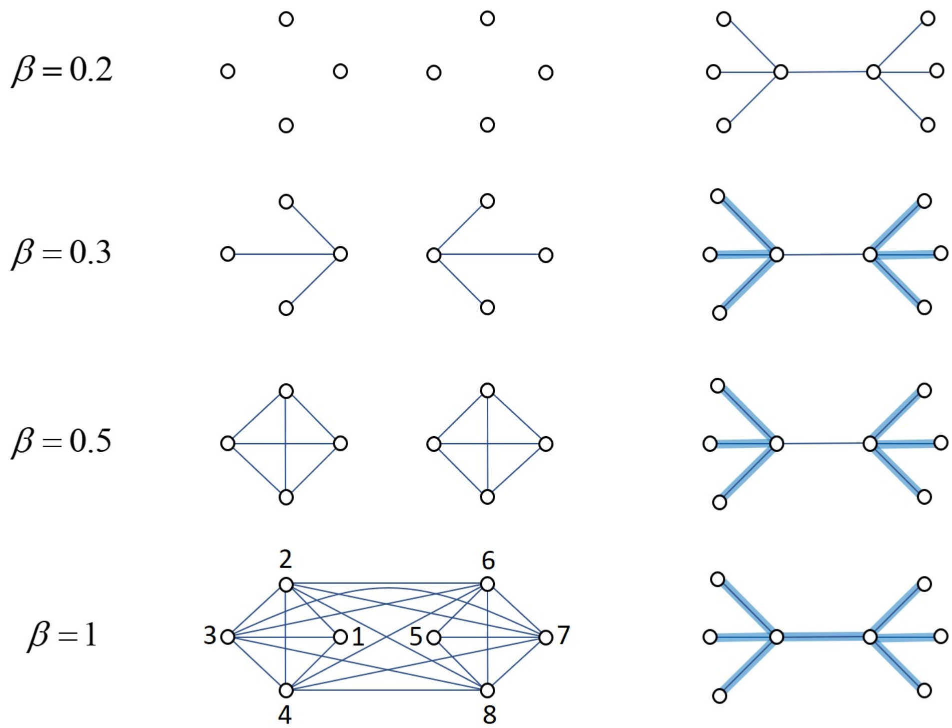


Figure 3.2: Communicability graphs (central panels) at different values of β for the tree Γ with degree sequence 4,4,1,1,1,1,1,1. In the right panel the edges of the Lindemann graphs are represented as solid lines over the edges of the original graph Γ.

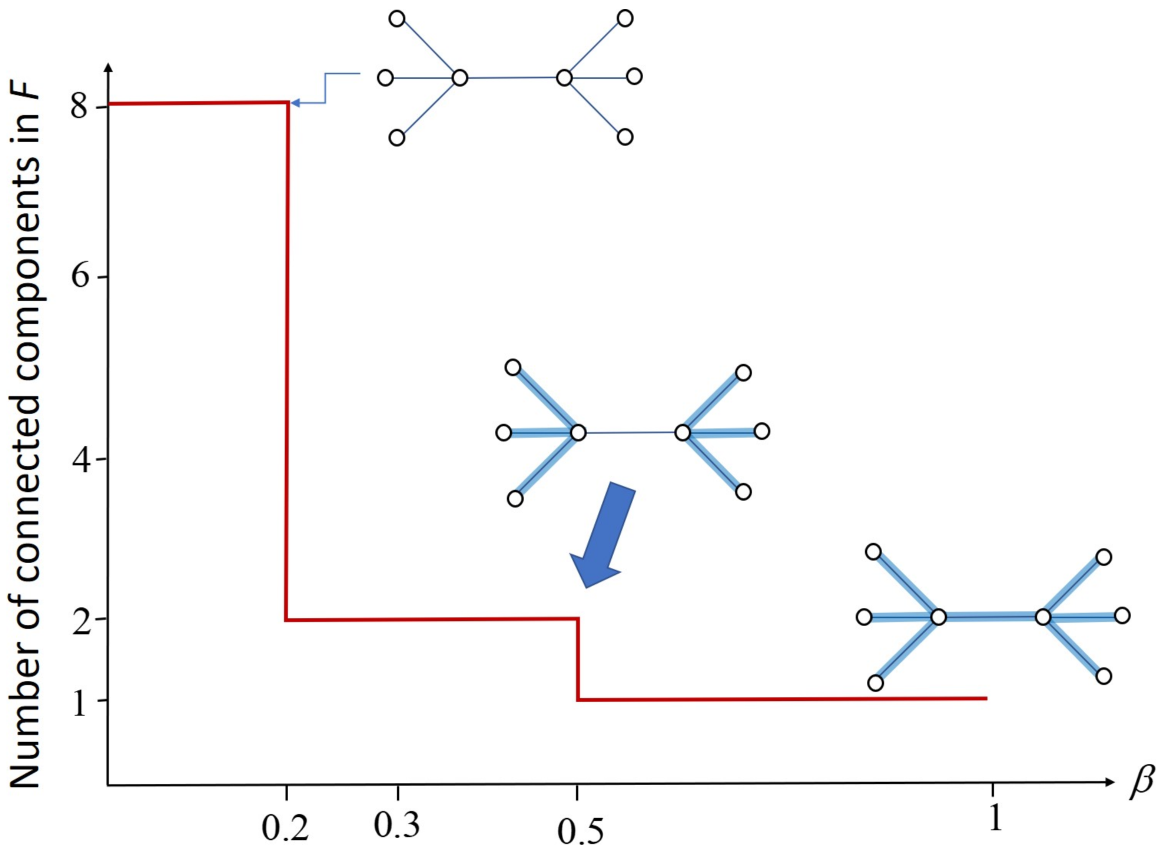


Figure 3.3: Illustration of the transition between connected $\beta > 0.5$ to disconnected $\beta \leq 0.5$ Lindemann graph as a function of β for the simple tree illustrated in Fig. 3.2.

4 Universality of the topological melting transition

Here we prove the existence of the phase transition between connected to disconnected Lindemann graph for any simple graph. For proving this result it is enough to prove that this transition occurs in the communicability graph. Then, when the communicability graph is connected also is the Lindemann graph, due to the fact that there is a path between every pair of nodes in a connected graph. In the same way, if the communicability graph is disconnected also is the Lindemann graph because there will be pairs of adjacent nodes of the original graph for which there are no paths connecting them in the communicability graph. We divide our result into two parts. The first deals with all graphs which are not complete multipartite ones. The second proves the result for this kind of graphs.

Theorem 11. *Let $H(\mathit{\Gamma},\beta)$ be the communicability graph for a non complete multipartite graph $\Gamma=(V,E)$. Then, there exist a value $\beta_c\in[0,\infty)$ such that*

(i) $H(\mathit{\Gamma},\beta\geq\beta_c)$ is connected;

(ii) $H(\mathit{\Gamma},\beta<\beta_c)$ is disconnected.

Proof. We start by proving that the communicability graph $H(\mathit{\Gamma},\beta)$ is disconnected for certain value of the inverse temperature. Then, we prove that it becomes connected for certain value of β, which immediately implies that the communicability graph $H(\mathit{\Gamma},\beta)$ makes a transition from connected to disconnected at certain intermediate temperature, which we call β_c. First, we prove that such transition from connected to disconnected is unique. In other words, we prove that once the graph become disconnected it will not reconnect again for any $\beta<\beta_c$. We will prove that the value of β_c is unique by proving that if $\triangle\tilde{G}_{pq}(\beta_c)\geq 0$, for $\beta_c\in[0,\infty)$, then it is also positive for any $\beta_2>\beta_c$. We recall that

$$\mathit{\Delta}\tilde{G}_{pq}(\beta):=M(\mathit{\Gamma},\beta)+\sum_{j=2}^{n}\psi_j(p)\,\psi_j(q)\,e^{\beta\lambda_j},\tag{4.1}$$

where $M(\mathit{\Gamma},\beta)=\max_{s\neq t\in V}\sum_{j=2}^{n}\psi_j(s)\,\psi_j(t)\,e^{\beta\lambda_j}$. Let us consider that for a given graph there is a value β_c for which $\triangle\tilde{G}_{pq}(\beta_c) \geq 0$, for all $p, q \in V$, which indicates that the Lindemann graph is connected. This is equivalent to say that

$$\sum_{j\geq 2}^{+} \psi_j(p)\psi_j(q)e^{\beta_c\lambda_j} + M(\Gamma, \beta_c) \geq \left| \sum_{j\geq 2}^{-} \psi_j(p)\psi_j(q)e^{\beta_c\lambda_j} \right|, \tag{4.2}$$

where the signs $+$ and $-$ in the sums indicate that the summations are carried out over positive and negative terms, respectively. Then, let us consider a value $\beta_2 = \beta_c + \epsilon > \beta_c$. Then we prove that the graph is connected for this value of β. That is, we prove that

$$\sum_{j\geq 2}^{+} \psi_j(p)\psi_j(q)e^{(\beta_c+\epsilon)\lambda_j} + M(\Gamma, (\beta_c + \epsilon)) \overset{?}{\geq} \left| \sum_{j\geq 2}^{-} \psi_j(p)\psi_j(q)e^{(\beta_c+\epsilon)\lambda_j} \right|. \tag{4.3}$$

From 4.2, we have

$$\left(\sum_{j\geq 2}^{+} \psi_j(p)\psi_j(q)e^{\beta_c\lambda_j} + M(\Gamma, \beta_c) \right) \left(\sum_{j=2}^{n} e^{\epsilon\lambda_j} \right) \geq \left| \sum_{j\geq 2}^{-} \psi_j(p)\psi_j(q)e^{\beta_c\lambda_j} \right| \left(\sum_{j=2}^{n} e^{\epsilon\lambda_j} \right), \tag{4.4}$$

which can be written in the form

$$\sum_{j\geq 2}^{+} \psi_j(p)\psi_j(q)e^{(\beta_c+\epsilon)\lambda_j} + M(\Gamma, (\beta_c + \epsilon)) + \left(\sum_{j\geq 2}^{+} \psi_j(p)\psi_j(q)e^{\beta_c\lambda_j} \right) \left(\sum_{k\neq j\geq 2} e^{\epsilon\lambda_k} \right) + M(\Gamma, \beta_c) \left(\sum_{k\neq j\geq 2} e^{\epsilon\lambda_k} \right) \geq$$
$$\left| \sum_{j\geq 2}^{-} \psi_j(p)\psi_j(q)e^{(\beta_c+\epsilon)\lambda_j} \right| + \left| \sum_{j\geq 2}^{-} \psi_j(p)\psi_j(q)e^{\beta_c\lambda_j} \right| \left(\sum_{k\neq j\geq 2} e^{\epsilon\lambda_k} \right),$$

Thus, we have

$$\sum_{j\geq 2}^{+} \psi_j(p)\psi_j(q)e^{(\beta_c+\epsilon)\lambda_j} + M(\Gamma, (\beta_c + \epsilon)) \geq \left| \sum_{j\geq 2}^{-} \psi_j(p)\psi_j(q)e^{(\beta_c+\epsilon)\lambda_j} \right|, \tag{4.5}$$

because

$$\left(\sum_{j\geq 2}^{+}\psi_j(p)\psi_j(q)e^{\beta_c\lambda_j}\right)\left(\sum_{k\neq j\geq 2}e^{\epsilon\lambda_k}\right)+M(\Gamma,\beta_c)\left(\sum_{k\neq j\geq 2}e^{\epsilon\lambda_k}\right)\geq\left|\sum_{j\geq 2}^{-}\psi_j(p)\psi_j(q)e^{\beta_c\lambda_j}\right|\left(\sum_{k\neq j\geq 2}e^{\epsilon\lambda_k}\right).$$

which proves that β_c is unique.

Now, we continue by proving the existence of this transition for any simple graph. Recall, that two distinct nodes $p \neq q$ are connected in $H(\Gamma, \beta)$ if $\triangle\tilde{G}_{pq} \geq 0$, and disconnected if $\triangle\tilde{G}_{pq} < 0$. Let us consider the case when $\beta = 0$. Thus,

$$\triangle\tilde{G}_{pq}\left(\beta=0\right)=-\left(\psi_1\left(p\right)\psi_1\left(q\right)+\max_{s\neq t}\psi_1\left(s\right)\psi_1\left(t\right)\right)<0. \tag{4.6}$$

Therefore, it is obvious that the edge pq in the graph is disconnected and this happens for every pair of nodes in the graph. Consequently, the communicability graph is disconnected for some β when $\beta \to 0$.

Let us now consider the case when $\beta \to \infty$. In this case the communicability function $\triangle\tilde{G}_{pq}(\beta)$ is dominated by the term containing the second largest eigenvalue λ_2. Now let $(r-1) \geq 1$ be the multiplicity of λ_2, i.e., $\lambda_2 = \lambda_3 = \cdots = \lambda_r$. Then, $\forall p, q \in V$, we have

$$\begin{aligned}\triangle\tilde{G}_{pq}(\beta) \quad&\rightarrow\quad (\psi_r\left(p\right)\psi_r\left(q\right)+\psi_{r-1}\left(p\right)\psi_{r-1}\left(q\right)+\ldots+\psi_2\left(p\right)\psi_2\left(q\right))e^{\beta\lambda_2}\\&\qquad+\max_{s\neq t}\left(\psi_r\left(s\right)\psi_r\left(t\right)+\psi_{r-1}\left(s\right)\psi_{r-1}\left(t\right)+\ldots+\psi_2\left(s\right)\psi_2\left(t\right)\right)e^{\beta\lambda_2},\end{aligned}$$

$$\Rightarrow\triangle\tilde{G}_{pq}(\beta)\rightarrow e^{\beta\lambda_2}\sum_{j=2}^{r}\psi_j\left(p\right)\psi_j\left(q\right)+e^{\beta\lambda_2}\max_{s\neq t}\sum_{j=2}^{r}\psi_j\left(s\right)\psi_j\left(t\right), \tag{4.7}$$

where $\psi_2, \psi_3, \ldots, \psi_{r-1}, \psi_r$, are the eigenvectors corresponding to the eigenvalue λ_2. If $\cap_{j=2}^{r}\mathcal{O}(\psi_j) \neq \emptyset$, then by Lemma 2, one of the following two separate cases hold.

Case 1. No edge in the original graph $\Gamma = (V, E)$ joins a vertex of $\mathscr{P}\left(\psi_j\right)$ to one of $\mathscr{N}\left(\psi_j\right)$. Then $\psi_j\left(p\right)\psi_j\left(q\right) \geq 0$, $\forall j \in \{2, 3, \ldots, r\}$, and $\forall (p, q) \in E$, $\triangle\tilde{G}_{pq}$ (4.7) satisfies:

$$\triangle\tilde{G}_{pq}(\beta)\geq 0. \tag{4.8}$$

Now let us rewrite the function $\triangle\tilde{G}_{pq}$ in the following form, where s and t are two distinct nodes in the graph:

$$\triangle\tilde{G}_{pq} = \left(\exp\left(\beta A\right)\right)_{pq} - \psi_1\left(p\right)\psi_1\left(q\right)e^{\beta\lambda_1} + \max_{s\neq t}\left[\left(\exp\left(\beta A\right)\right)_{st} - \psi_1\left(s\right)\psi_1\left(t\right)e^{\beta\lambda_1}\right].$$

Let us now consider $\beta = 0$, then $\forall p \neq q \in V$,

$$\triangle\tilde{G}_{pq} = -\psi_1\left(p\right)\psi_1\left(q\right) + \max_{s\neq t}\left[-\psi_1\left(s\right)\psi_1\left(t\right)\right] < 0, \tag{4.9}$$

since the leading eigenvector $\vec{\psi}_1$ can be chosen such that its components $\psi_1(p)$ are positive for all $p \in V$ according to the Perron-Frobenius theorem. The exponential matrix $\exp(0 \cdot A) = I$, so that $(\exp(\beta A))_{pq} = 0$, $\forall p \neq q \in V$. Then, from 4.8 and 4.9, we have that there is a value of $\beta_c \in [0, \infty)$, such that $H\left(\mathit{\Gamma}, \beta \geq \beta_c\right)$ is connected and $H\left(\mathit{\Gamma}, \beta < \beta_c\right)$ is disconnected.

Case 2. There exists at least one edge that joins a vertex of $\mathscr{P}(\psi_j)$ to one of $\mathscr{N}(\psi_j)$. Moreover, $\langle\mathscr{P}(\psi_j)\rangle$ and $\langle\mathscr{N}(\psi_j)\rangle$ are connected.

Let $p \in \cap_{j=2}^{r}\mathcal{O}(\psi_j)$, then $\psi_j\left(p\right) = 0$, $\forall j \in \{2, 3, \ldots, r\}$. Then $\forall q \neq p \in V$, we get:

$$e^{\beta\lambda_2}\sum_{j=2}^{r}\psi_j\left(p\right)\psi_j\left(q\right) = 0,$$

and

$$\triangle\tilde{G}_{pq}(\beta) \geq 0. \tag{4.10}$$

Therefore, all the nodes of V are connected to each other through p. Thus, from 4.9, and 4.10, we have that $\exists\beta_c \in [0, \infty)$, such that $H\left(\mathit{\Gamma}, \beta \geq \beta_c\right)$ is connected and $H\left(\mathit{\Gamma}, \beta < \beta_c\right)$ is disconnected.

Now let us consider the case in which $\cap_{j=2}^{r}\mathcal{O}(\psi_j) = \emptyset$. Let $p \in \mathscr{P}(\psi_j) \cup \mathcal{O}(\psi_j)$ (resp., $p \in$

$\mathscr{N}(\psi_j))$ $j \in \{2,3,\dots,r\}$. Then according to Lemma 3, there exists $q \in \mathscr{P}(\psi_j) \cup \mathcal{O}(\psi_j)$ (resp., $q \in \mathscr{N}(\psi_j))$ such that $(p,q) \in E$ and either $p,q \in \mathscr{P}(\psi_j) \cup \mathcal{O}(\psi_j)$ or $\mathscr{N}(\psi_j)$, $\forall j \in \{2,\dots,r\}$. It holds that $\psi_j(p)\,\psi_j(q) \geq 0$, $\forall j$ such that we get:

$$\sum_{j=2}^{r} \psi_j(p)\,\psi_j(q) \geq 0,$$

and

$$\triangle \tilde{G}_{pq}(\beta) \geq 0. \tag{4.11}$$

Now, since there are $(r-1)$ eigenvectors corresponding to the eigenvalue λ_2, there are 2^{r-1} intersected subsets in V of $\mathscr{P}(\psi_j) \cup \mathcal{O}(\psi_j)$ and $\mathscr{N}(\psi_j)$. In these sets the nodes have the same signs of the eigenvector components ψ_j, $\forall j \in \{2,3,\dots,r\}$. Let us denote these subsets by $W_1, W_2, \cdots, W_{2^{r-1}}$ (when $r-1=2$ these subsets are: $W_1 = (\mathcal{P}(\psi_2) \cup \mathcal{O}(\psi_2)) \cap (\mathcal{P}(\psi_3) \cup \mathcal{O}(\psi_3))$, $W_2 = (\mathcal{P}(\psi_2) \cup \mathcal{O}(\psi_2)) \cap \mathscr{N}(\psi_3)$, $W_3 = \mathscr{N}(\psi_2) \cap (\mathcal{P}(\psi_3) \cup \mathcal{O}(\psi_3))$ and $W_4 = \mathscr{N}(\psi_2) \cap \mathscr{N}(\psi_3)$). Then $\forall p,q \in W_h$, $\forall h \in \{1,2,\dots,2^{r-1}\}$, it holds that $\psi_j(p)\,\psi_j(q) \geq 0$, $\forall j$ and $\triangle \tilde{G}_{pq}(\beta) \geq 0$. So that the subgraph $\langle W_h \rangle$, $\forall h \in \{1,2,\dots,2^{r-1}\}$, is connected.

Finally, we need to show whether the subgraphs $\langle W_1 \rangle, \langle W_2 \rangle, \cdots, \langle W_{2^{r-1}} \rangle$ are connected to each other, such that we get a connected graph. Let $p' \in \langle W_h \rangle$ and $q' \in \langle W_s \rangle$, where $h, s \in \{1,2,\dots,2^{r-1}\}$, such that the absolute value of $\sum_{j=2}^{r} \psi_j(p')\,\psi_j(q')$, satisfies:

$$\sum_{j=2}^{r} \psi_j\left(p'\right) \psi_j\left(q'\right) \leq \max_{s \neq t \in V} \sum_{j=2}^{r} \psi_j(s)\,\psi_j(t),$$

Then $\triangle \tilde{G}_{p'q'}$ (4.7) satisfies:

$$\triangle \tilde{G}_{p'q'}(\beta) \geq 0, \tag{4.12}$$

therefore $\langle W_1 \rangle, \langle W_2 \rangle, \cdots, \langle W_{2^{r-1}} \rangle$ are connected to each other. Therefore, from 4.9, 4.11 and 4.12 we have that there is a $\beta_c \in [0,\infty)$, such that $H(\mathit{\Gamma}, \beta \geq \beta_c)$ is connected and $H(\mathit{\Gamma}, \beta < \beta_c)$

is disconnected, which finally proves the result. □

In the case of complete multipartite graphs which were not included in the Theorem 11 we have the following. As in the general case $\Delta\tilde{G}_{pq}(\beta \to 0) < 0$, which indicates that the edge does not exist, and this is true for any pair of nodes in the graph. Then, we have to show when such edge exists. According to Lemma 1 [24] in complete multipartite graphs $\lambda_2 \leq 0$. Then, let us first consider the case when $\lambda_2 = 0$. In this case when $\beta \to \infty$, the communicability function $\triangle\tilde{G}_{pq}(\beta)$ is dominated by the term of the largest eigenvalue λ_2. Now let $(r-1) \geq 1$ be the multiplicity of λ_2, i.e., $\lambda_2 = \lambda_3 = \cdots = \lambda_r$. Then $\forall p, q \in V$,

$$\triangle\tilde{G}_{pq}(\beta) \quad \to \quad e^{\beta\lambda_2} \sum_{j=2}^{r} \psi_j\left(p\right)\psi_j\left(q\right) + e^{\beta\lambda_2} \max_{s\neq t\in V} \sum_{j=2}^{r} \psi_j\left(s\right)\psi_j\left(t\right),$$

which implies that

$$\triangle\tilde{G}_{pq}(\beta) \to \sum_{j=2}^{r} \psi_j\left(p\right)\psi_j\left(q\right) + \max_{s\neq t\in V} \sum_{j=2}^{r} \psi_j\left(s\right)\psi_j\left(t\right), \tag{4.13}$$

since $e^{\beta\lambda_2} = 1$. So that the proof for the case when $\cap_{j=2}^{r}\mathcal{O}(\psi_j) \neq \emptyset$, will be the same as that for the case when $\lambda_2 > 0$, which is the Case 2, in Theorem 10.

Now when $\cap_{j=2}^{r}\mathcal{O}(\psi_j) = \emptyset$ then for the nodes which belong to the sets W_h, $\forall h \in \{1, 2, \ldots, 2^{r-1}\}$, (the sets of all of intersected subsets in V of $\mathscr{P}(\psi_j) \cup \mathcal{O}(\psi_j)$ and $\mathscr{N}(\psi_j)$, $j \in \{2, 3, \ldots, r\}$) are connected to each other in $\langle W_h \rangle$, since they have the same signs of the eigenvector components ψ_j, $\forall j \in \{2, 3, \ldots, r\}$. For the nodes which do not belong to W_h, $\forall h \in \{1, 2, \ldots, 2^{r-1}\}$, let $p \in V$, $p \notin W_h$, $\forall h \in \{1, 2, \ldots, 2^{r-1}\}$, and let $q \in W_h$, such that the absolute value of $\sum_{j=2}^{r} \psi_j\left(p\right)\psi_j\left(q\right)$, satisfies

$$\left| \sum_{j=2}^{r} \psi_j\left(p\right)\psi_j\left(q\right) \right| \leq \max_{s\neq t\in V} \sum_{j=2}^{r} \psi_j\left(s\right)\psi_j\left(t\right),$$

Then $\triangle\tilde{G}_{pq}$ (4.13) satisfies

$$\triangle\tilde{G}_{pq}(\beta) \geq 0. \tag{4.14}$$

So let us denote the subgraphs generated by W_h, and the other nodes of V which do not belong to W_h, by $\langle W_1' \rangle, \langle W_2' \rangle, \cdots, \left\langle W_{2^{r-1}}' \right\rangle$. Finally, in the same previous way we can connect $\langle W_1' \rangle, \langle W_2' \rangle, \cdots, \left\langle W_{2^{r-1}}' \right\rangle$ to each other, such that we get a connected graph. Let $p' \in \langle W_h' \rangle$ and $q' \in \langle W_s' \rangle$, where $h, s \in \{1, 2, \ldots, 2^{r-1}\}$, such that the absolute value of $\sum_{j=2}^{r} \psi_j(p')\psi_j(q')$, satisfies:

$$\left| \sum_{j=2}^{r} \psi_j\left(p'\right)\psi_j\left(q'\right) \right| \leq \max_{s \neq t \in V} \sum_{j=2}^{r} \psi_j(s)\psi_j(t).$$

Therefore, $\triangle\tilde{G}_{pq}$ (4.13) satisfies

$$\triangle\tilde{G}_{p'q'}(\beta) \geq 0. \tag{4.15}$$

Consequently $\langle W_1' \rangle, \langle W_2' \rangle, \cdots, \left\langle W_{2^{r-1}}' \right\rangle$ are connected to each other. Thus, from 4.9, 4.14 and 4.15 we have that there is $\beta_c \in [0, \infty)$, such that $H(\mathit{\Gamma}, \beta \geq \beta_c)$ is connected and $H(\mathit{\Gamma}, \beta < \beta_c)$ is disconnected.

On the other hand, when $\lambda_2 < 0$ we have that

$$\mathit{\Delta}\tilde{G}_{pq}(\beta) = \max_{s \neq t} \sum \psi_j(s)\psi_j(t)e^{-\beta|\lambda_j|} + \sum_{j=2}^{n} \psi_j(p)\psi_j(q)e^{-\beta|\lambda_j|}. \tag{4.16}$$

This means that $\lim_{\beta\to\infty} \mathit{\Delta}\tilde{G}_{pq}(\beta) = 0$. However, such limit can be either positive–existence of the edge–or negative–not existence of the edge. Thus, in this case we can consider that the edge exists if $\left|\lim_{\beta\to\infty} \mathit{\Delta}\tilde{G}_{pq}(\beta)\right| \leq \varepsilon$, where ε is a threshold very close to zero. The case of complete multipartite graphs is an all-or-nothing case of melting. That is, at $\beta = 0$ all the nodes in the Lindemann graph are isolated. When β is very large all the nodes in the communicability graph are connected to each other and the Lindemann graph is the same as the original graph. Thus, in these graphs there is not a gradual melting as in the rest of the other graphs, but there is an abrupt transition between being connected to fully disconnected.

5 Melting of granular materials

In this section we study the influence of order and randomness on the melting phase transition in granular materials. The influence of order vs. randomness is on the basis of many physical problems. In particular, here we are interested in studying the differences in the topological melting of granular materials with ordered structures vs. those having random ones. The classical example of an ordered system is a crystal where granular particles are arranged in a repeating pattern [26]. On the other hand, amorphous solids, which are characterized by the lack of regular pattern or repetition, are good examples of random-like materials [1]. In order to model a random-like granular material we consider here a type of random graph known as the Gabriel graph [12]. The Gabriel graphs $\Gamma = (V, E)$ are constructed by placing randomly and independently n points in a unit square, then for each pair of points $i \in V$, $j \in V$, $i \neq j$, constructs a disk in which the line segment $\overline{ij}$ is a diameter (see Fig. 5.1 (left panel)). The two points will be connected if the corresponding disk does not contain any other element of V. An example of Gabriel graph is given in Fig. 5.1 (Right panel).

The reason why we consider random neighborhood (Gabriel) graphs here instead of other types of random graphs is the following. To keep the analogy with solid granular materials we should maintain certain geometric disposition of the nodes. This geometric arrangements of nodes are possible in the so-called random geometric graphs (RGGs) as well as in the random neighborhood graphs (RNGs). The RGGs are nonplanar graphs, which implies that node A can interact with another B even in the case that a third node C is exactly in the middle between A and B. This, of course, is not a realistic scenario for the interaction between granular particles and not appropriate for representing a granular material. However, Gabriel graphs are planar graphs and avoid the interaction between mutually occluded nodes. Consequently, they are appropriate to model amorphous granular materials.

The differences in the ordered vs. random arrangement of particles in crystalline and

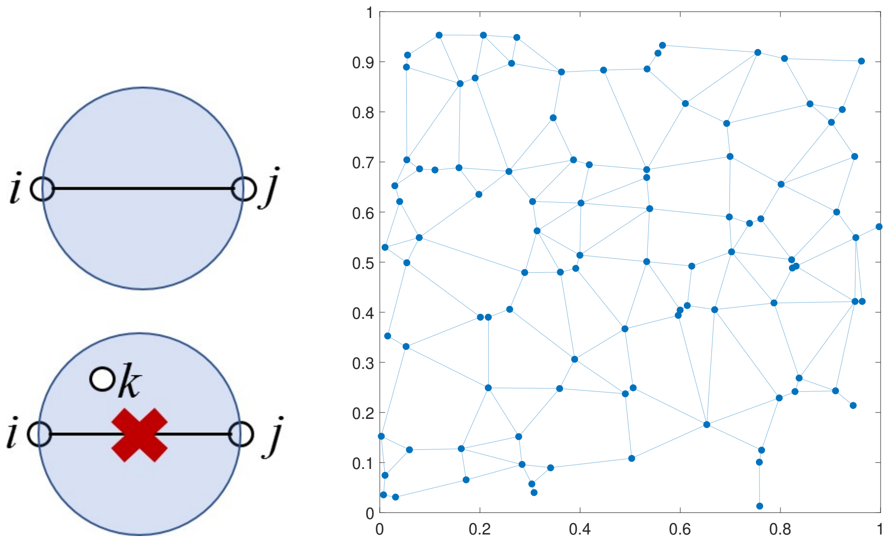


Figure 5.1: Illustration of the construction process of a Gabriel graph (left), where a disk is defined for a pair of nodes which forms a diameter of the disk. Because there is no point inside that disk the two nodes are connected (top graphic). In the bottom graphic a point k is inside the disk and the two nodes i and j are not connected. (right panel) An example of a Gabriel graph with $n = 100$ nodes.

amorphous granular materials make that they differ significantly in the way they change their phase from solid to liquid. That is, a fundamental difference between crystalline and amorphous solids resides in the way they melt. While a crystalline solid has a sharp transition from solid to liquid, the amorphous solid does not. Instead, it displays a very smooth transition for a long range of temperatures. The second characteristic feature is that for the same material in amorphous and crystalline forms, the amorphous one melts at higher temperature than the crystalline one. For instance, crystalline quartz melts at $1,550°C$ and amorphous quartz melts in the range $1,500-2,000°C$. We are interested in investigating here this physical reality as an analogy for our crystalline and amorphous granular material graphs.

In Fig. 5.2 we illustrate the plot of the change in the number of connected components in the communicability graph with the change of β for a 10×10 square grid and a Gabriel graph with $n = 100$ nodes and $m = 180$ edges. Similar results to the ones presented here were obtained for triangular and hexagonal lattices (results not shown). The main difference between these two kinds of graphs studied here resides only in the order/randomness of the

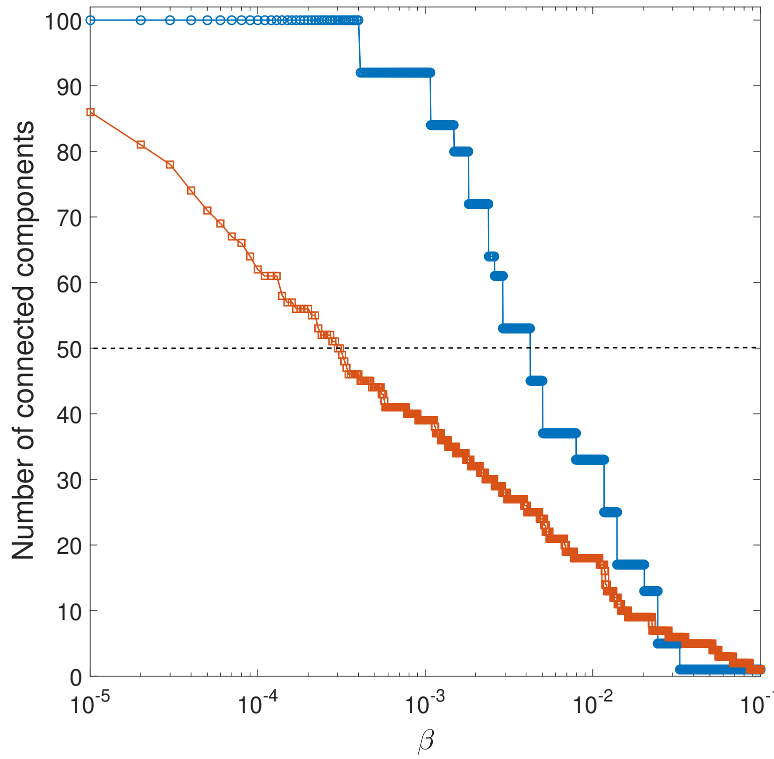


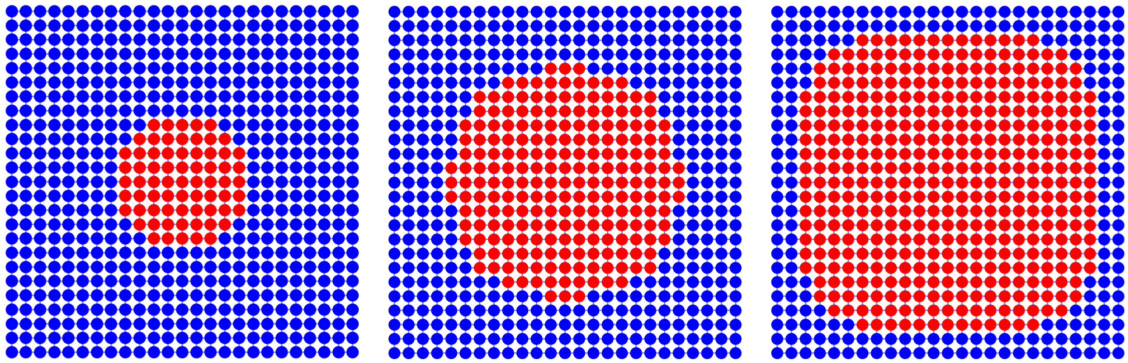
Figure 5.2: Change of the number of connected components in the Lindemann graph for the 10×10 square grid (circles) and Gabriel graph with $n = 100$ nodes and $m = 180$ edges (squares). The results for the Gabriel graphs are the average of 100 random realizations.

nodes in a unit square. The lattice representing a crystalline granular material and the Gabriel graph representing an amorphous one. The main observation is that while the crystalline granular material displays a sharp increase in the number of connected components with the decrease of β–a sharp melting transition–, the amorphous one displays a rather slow change (notice that the x-axis is in logarithmic scale)–slow melting transition. The second important observation is that the structure of the crystalline graph is destroyed more quickly than that of the amorphous one. For instance, if we consider the value of β at which the number of connected components is exactly half the number of nodes, we can see that the crystalline graph reaches that point an order of magnitude before than the amorphous one. We repeated the experiment with a 25×25 square lattice and the corresponding Gabriel graph to see whether there are some small size effects and observed that the results are very much the same, although we have increased the size of the graphs by a factor of 6 (results not shown).

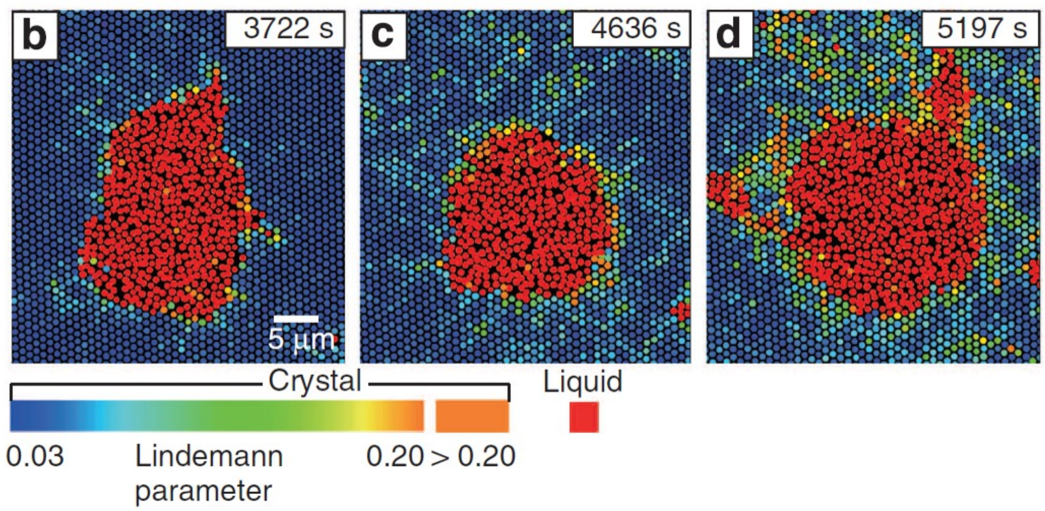
Another possibility of the current approach is that it allows us to visualize the evolution of the “topological melting” process in granular materials in order to gain insights about its mechanism. In Fig. 5.2 we illustrate some snapshots of the change in the communicability structure with the change of β for the square lattice. We represent in red the nodes for which all of their edges have been removed, and which are disconnected from the giant connected component, i.e., those particles which are in the liquid state. In blue we represent those nodes which form the giant connected component of the graph, i.e, still in the solid phase.

At very low values of β, e.g. $\beta = 0.000025$ (Fig. 5.3 (c)) the communicability structure of the lattice resembles a trivial graph in which almost every node is isolated, i.e., the whole material is in the liquid state. As the temperature drops, β increases, certain structures start to emerge, i.e., island of solid structures. In particular, for $\beta = 0.0005$ (Fig. 5.3 (b)) an annulus–external part of the lattice–is solidified into a single connected component and only the central part of the granular material remains melted. As the temperature drops below $\beta = 0.000075$ (Fig. 5.3 (a)), the melted region–red nodes–shrinks to the very center of the lattice. The observed pattern of melting of the square lattice is similar to the one observed experimentally for crystalline granular (colloidal) material. In Fig. (Fig. 5.3 (d)) we illustrate the results of Wang et al. [28] for the melting of colloidal crystals which show such pattern of central melting.

In the case of the amorphous granular materials there is no repeating pattern in them, and it is difficult to find a general structural pattern of the evolution of the melting process. A few snapshots of the process are given in Fig. 5.4. The temperature needed to melt these graphs is significantly higher–smaller β–than the ones needed to melt square lattices of the same size, which coincides with our previous observations as well as with the experimental results for crystalline and amorphous solids.



(a) (b) (c)



(d)

Figure 5.3: Illustration of the melting of a 25 × 25 square lattice at $\beta = 0.000075$ (a), $\beta = 0.00005$ (b) and $\beta = 0.000025$ (c). Results for the melting of colloidal crystals obtained by Wang et al. [28]. In plots (a)-(c) the nodes not in the giant connected component are colored in red.

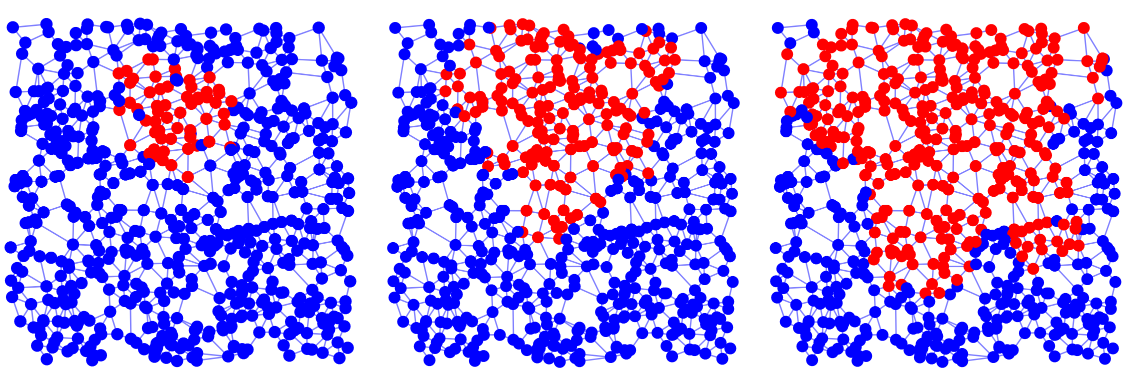


Figure 5.4: Nodes in each of the connected components of the Gabriel graph studied here for $\beta = 10^{-8}$, 10^{-9} and 10^{-10} from left to right. The nodes not in the giant connected component are colored in red.

6 Summary

The most important result of the current work is the proof of the existence of a universal topological melting transition in graphs. This transition takes place when we consider a Lindemann-like model on graphs, which is based on a vibrational approach of nodes and edges. From a mathematical point of view the current method is based on the spectral properties of the adjacency matrix of the graph and the changes taking place on the exponential matrix function $\exp(\beta A)$ with the changes of β. In this way, regular-like graphs like square lattices are easier to melt than more irregular structures, such as spatial random graphs. These differences resemble the known dissimilarities between crystalline and amorphous granular materials in their melting.

The current model of melting could resemble a kind of percolation process [6]. However, the melting phenomenon considered here is driven by the parameter β which acts as a thermal bath for all the network, and is not directly related to site or bond percolation, that are processes that act at a local level, even core percolation processes [16] maintain a sort of locality. In this sense the process described here is more similar to a "global degradation" of the full connectivity of the network [4], proposed as a model for the better understanding of the mechanistic effects of the Alzheimer disease. Although we have not considered a statistical mechanics approach in this work it is worth mentioning here that the transition observed here is similar to a kind of continuous transition with discontinuities [18], exhibiting infinitely many discontinuous jumps in an arbitrary vicinity of the transition point.

The analysis of graph melting as proposed here opens many new possibilities for the study of granular materials. There are many mathematical and computational questions that remain open from the current study. They include, but are not limited, to the following ones: (i) A more exhaustive analysis of the topological drivers of the graph melting; (ii) How certain specific topological properties of graphs influence the melting temperature and the melting process of granular materials?; (iii) Is there a general statistical mechanics formulation of this process? We hope the reader can help to answer some of these questions and generate new ones that clarify our understanding of granular materials represented by graphs.

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